Ethan Curtis

curtie@stanford.edu
380 Roth Way, Stanford, CA 94305

Educational Background

Stanford University **Summer 2019 – present**
Ph.D., Theoretical Chemistry
Research Advisor: Todd Martínez

University of Michigan, Ann Arbor **Fall 2015 – Spring 2019**
B.S.Chem., Honors Chemistry and Honors Mathematics
Research Advisor: Paul Zimmerman

- Graduated with High Distinction; High Honors in Chemistry, and Honors in Math

Research Experience

Graduate Student, Martínez Lab **Summer 2019 – Present**

- Writing a python package for automated single-molecule forcefield fitting using an iterative method to augment the training dataset
- Examining how to generate initial conditions for excited-state dynamics (and spectra) for QM/MM systems
- Studying the excited-state dynamics of Donor-acceptor Stenhouse adduct crystals using an *ab initio* exciton model and *ab initio* multiple spawning
- Estimating basis set superposition error using empirical methods and neural networks
- Helped write GPU-accelerated coupled-cluster code for TeraChem, the Martínez lab's GPU-accelerated quantum chemistry package

Undergraduate member, Zimmerman Lab **Fall 2015 – Fall 2019**

- Investigated the kinetics and thermodynamics of the Schlenk equilibrium with respect to thiophene Grignards

Multidisciplinary Design Program **Winter 2018 – Winter 2019**

- Worked with a team of chemistry and engineering students to develop and test an end-to-end method for extraction, refinement, and 3D printing of structural material in non-terrestrial environments
- Results presented at ASGSR Fall 2018 meeting, to NASA Space Technologies Mission Directorate, and to the Chief Technology Council of Northrop Grumman

Oklahoma State University REU Program **Summer 2018**

- Worked in the Fennell lab developing classical water models by trying to incorporate polarization effects

Publications

- **E. Curtis**, C. Jones, T. Martínez. "Preparing initial conditions for excited-state dynamics in solvated systems." *In prep.*
- **E. Curtis**, T. Martínez. "Iterative forcefield optimization using validation sets and accelerated sampling methods." *In prep.*
- B. S. Fales, **E. Curtis**, K. G. Johnson, D. Lahana, S. Seritan, Y. Wang, H. Weir, T. Martínez, E. Hohenstein. "Performance of Coupled-Cluster Singles and Doubles on Modern Stream Processing Architectures." *J. Chem. Theory Comput.* **2020,** 16 (7), 4021-4028.
- **E. Curtis**, M. Hannigan, A. Vitek, P. Zimmerman. "Quantum Chemical Investigation of Dimerization in the Schlenk Equilibrium of Thiophene Grignard Reagents." *J. Phys. Chem. A,* **2020,** 124 (8), 1480-1488.

Poster Presentations

- **E. Curtis**, T. Martínez. "Automated Force Field Fitting: Toward a Black Box Approach." *American Conference on Theoretical Chemistry* (2022).
- **E. Curtis**, E. Taffet, T. Martínez. "Excitonic Photochemistry of Donor-Acceptor Stenhouse Adducts Modeled in the Molecular Crystal." *Bay Area Theoretical Chemistry Conference* (2021).
- **E. Curtis**, U. Raucci, D. Sanchez, E. Taffet, C. Punwong, T. Martínez. "Examining the Excited State Dynamics of DASA Aggregates." *Virtual Conference on Theoretical Chemistry* (2020).
- **E. Curtis**, Z. Bellar, A. Chow, A. Kang, S. Sanvordenkar, G. Schlain, A. Wang, S. Maldonado. "Applications of in situ Additive Manufacturing on Mars." *American Society for Gravitational and Space Research* (2018). **Poster award**
- **E. Curtis**, C. Fennell. "Representing Water by Mixing Water Models." *Oklahoma State University Summer Undergraduate Research Symposium* (2018).
- **E. Curtis**, A. Vitek, P. Zimmerman. "Computing the Schlenk Equilibrium for Thiophene Grignards." *255th American Chemical Society National Meeting* (2018). **Poster award**
- **E. Curtis**, A. Vitek, P. Zimmerman. "Computational Investigation of the Schlenk Equilibrium for Thiophene Grignards." *University of Michigan Summer Undergraduate Research Symposium* (2017).
- **E. Curtis**, A. Vitek, P. Zimmerman. "Computational Investigation of Ring-walking on a Substituted Phenylene Tetramer." *Notre Dame Summer Undergraduate Research Symposium* (2016).

Teaching Experience

Teaching Assistant, Stanford Chemistry Department **Fall 2019 – Winter 2021**

- Winter 2021: Chem 151, Inorganic Chemistry I
  - Head TA
  - Designed problem sets and computer exercises
  - Led one hour recitation section each week
- Fall 2020: Chem 33, Organic Chemistry I
  - Worked with professor to write and edit weekly quizzes and exams
  - Administered, graded (and regraded) weekly quizzes and exams
- Winter 2020: Chem 151, Inorganic Chemistry I
  - Designed problem sets and computer exercises
  - Led one hour recitation section each week
- Fall 2019: Chem 121, Organic Chemistry II
  - Led two three-hour labs each week

Technical Skills

- C, C++, Python, Java, BaSH
- Q-Chem, TeraChem, Amber, Gaussian, Gromacs,
- PyTorch, Tensorflow, RDKit